

Abstract No. maro339

Biological Metal Clusters: Biophysical and Model Studies

M. Maroney (U. Of Massachusetts), S. Ragsdale (U. Of Nebraska), P. Carrington (U. Of Massachusetts), Y-C. Horng (U. Of Nebraska), P. Bryngelson and F. Al-Mjeni (U. Of Massachusetts)

Beamline(s): X9B

ABSTRACT: Methylcoenzyme M reductase (MCR) is the enzyme that catalyzes the last step of methanogenesis. This reaction involves a Ni tetrapyrrole cofactor called F_{430} . The redox chemistry of this cofactor has been the subject of considerable study and debate. We have monitored the redox chemistry involved in the interconversion of three states: resting (Ni(II)), Ox 1 and Red 1. XANES analysis show that all three forms are likely to contain six-coordinate Ni centers. Monitoring the Ni K-edge energy reveals small changes that indicate that both Ox 1 and Red 1 contain reduced Ni centers. The analysis of EXAFS features due to scattering from atoms in the macrocycle indicate that large changes in the conformation of the macrocycle, as suggested by other researchers, are not involved. The work continues with an effort being made to identify the axial ligands involved.